Devising Treasure Maps for Thermoelectrics and Topological Insulators

In the last decade, two major trends have emerged in Materials Science. On the one hand, ab-initio based simulations are increasingly employed to compute the properties of advanced functional materials. On the other hand, techniques of combinatorial materials synthesis are utilized to efficiently produce and optimize novel materials. Here we push for a third strategy to identify and improve advanced materials, in particular compounds with special thermoelectric properties and materials, which act as topological insulators. In this approach, a fundamental understanding of the relationship between structure and bonding and the resulting material properties will be utilized to establish 'treasure' maps, which relate desired properties to the composition of the material. In particular, we want to apply the concept of a 'treasure' map to other important and technologically relevant materials such as thermoelectrics and topological insulators. To draw a treasure map, the set of coordinates to obtain separation of the desired property (i.e. thermoelectricity, TI-ness) is crucial. It is therefore important that the underlying cause of the property is reflected in coordinates, and the properties of the chemical bonding that produce the desired materials function are robust. The goal of our work is thus to develop and utilize a fundamental understanding of the relationship between composition, bonding and atomic arrangement and the resulting material properties.